Crystal structure of diytterbium palladium hexagermanide, Yb_2PdGe_6

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Abstract

Ge_6PdYb_2 , orthorhombic, *Cmca* (No. 64), $a = 8.142(2)$ Å, $b = 7.980(2)$ Å, $c = 21.829(3)$ Å, $V = 1418.3$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.027$, $wR_{\text{obs}}(F^2) = 0.060$, $T = 293$ K.

Source of material

The title compound has been synthesized by induction melting stoichiometric amounts of ytterbium (99.9%), palladium (99.9%) and germanium (99.999%) in a tantalum crucible sealed by arc welding under argon. The sample was then closed in a quartz tube under vacuum and annealed at 1013 K for 24 days.

Discussion

The compound Yb_2PdGe_6 was determined by powder diffraction as crystallizing with the Ce_2CuGe_6 type [1,2]. In the present work, a study by single-crystal methods revealed a larger cell with double

a and c lattice parameters and an atomic arrangement very similar to the $\text{Ce}_2(\text{Ge}_{0.9}\text{Ga}_{0.1})_7$ structure [3]. The Yb_2PdGe_6 structure represents an ordered derivative. The structure of $\text{Ce}_2(\text{Ge}_{0.9}\text{Ga}_{0.1})_7$ is a vacancy variant of ScNiSi_3 and can be considered as an intergrowth of fragments of the AlB_2 , BaAl_4 and α -Po types along the c direction [3]. It was also discussed as member of a family of related structures by Zhao *et al.* [4]. In the figure, only half unit cell is drawn along the a axis, the full circles being atoms at $x = 0$ and the open circles being atoms at nearly $x = -1/4$ and $1/4$. In the AlB_2 fragment, ytterbium trigonal prisms (light stippling) are centred by the Ge2 and Ge3 atoms. The BaAl_4 fragment bears the square antiprisms with composition Yb_4Ge_4 around Pd (dark stippling). However, a deformation in the Ge—Ge distances involving the Ge1, Ge4 and Ge5 atoms along both a and b axes does not allow to fill all square antiprismatic voids, so that occupied polyhedra alternate with empty ones. The deformation is evident also in the α -Po fragment, where rows of distorted Ge cubes are found. All Ge atoms are surrounded by trigonal prisms. They are formed by $2\text{Yb} + 4\text{Ge}$ atoms with two lateral faces capped by one Ge and one Pd atom for Ge1, Ge4 and Ge5, but are formed by 6Yb for Ge2 (with two lateral faces capped by Ge) and Ge3 (with all three lateral faces capped by $2\text{Ge} + 1\text{Pd}$). The square antiprism around Pd is completed by a Ge atom capping the largest square face. The shortest interatomic distances are $d(\text{Ge3—Ge3}) = 2.447(9)$ Å, $d(\text{Pd—Ge3}) = 2.449(1)$ Å and $d(\text{Yb—Ge2}) = 2.972(4)$ Å, reaching a 10%–11% contraction with respect to the appropriate sum of the metallic radii for CN12 [5].

Table 1. Data collection and handling.

Crystal:	metallic grey prism, size $0.04 \times 0.08 \times 0.10$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71069 Å)
μ :	534.95 cm^{-1}
Diffractionmeter, scan mode:	Nonius MACH3, ω
$2\theta_{\text{max}}$:	59.88°
$N(hkl)_{\text{measured}}, N(hkl)_{\text{unique}}$:	1091, 1091
Criterion for $I_{\text{obs}}, N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 674
$N(\text{param})_{\text{refined}}$:	50
Programs:	SHELXS-97 [6], SHELXL-97 [7], STRUCTURE TIDY [8]

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Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Yb	16g	0.24954(4)	0.3754(2)	0.08257(1)	0.0025(2)	0.0064(2)	0.0079(2)	−0.0007(1)	0.0003(1)	−0.0001(7)
Pd	8f	0	0.1264(1)	0.14140(4)	0.0016(3)	0.0058(3)	0.0054(3)	0	0	0.0001(4)
Ge(1)	16g	0.27580(9)	0.1262(4)	0.19377(3)	0.0033(3)	0.0064(3)	0.0078(3)	−0.0001(9)	−0.0011(2)	−0.0002(6)
Ge(2)	8f	0	0.1205(6)	0.46047(6)	0.0064(5)	0.0059(6)	0.0134(5)	0	0	−0.000(1)
Ge(3)	8f	0	0.1308(7)	0.02925(5)	0.0094(5)	0.0055(6)	0.0051(4)	0	0	−0.0003(8)
Ge(4)	8f	0	0.3478(2)	0.30681(6)	0.0029(5)	0.008(1)	0.0076(5)	0	0	−0.0008(5)
Ge(5)	8f	0	0.4044(2)	0.19408(6)	0.0030(5)	0.0050(9)	0.0077(5)	0	0	−0.0020(4)

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References

1. Seropegin, Yu. D.; Borisenko, O. L.; Bodak, O. I.; Nikiforov, V. N.; Kovachikova, M. V.; Kochetkov, Yu. V.: Investigation of phase relationships and physical properties of Yb–Pd–Ge compounds. *J. Alloys Compd.* **216** (1994) 259–263.
2. Sologub, O.; Hiebl, K.; Rogl, P.; Bodak, O. I.: Formation, crystal chemistry and magnetism of compounds RE₂TGe₆, RE = rare earth, T = Pd, Pt, Cu, Ag and Au. *J. Alloys Compd.* **227** (1995) 37–39.
3. Yarmolyuk, Ya. P.; Pecharskii, V. K.; Gryniv, I. A.; Bodak, O. I.; Zavodnik, V. E.: Crystal structure of Ce₂(Ge_{0.9}Ga_{0.1})₇. *Sov. Phys. Crystallogr.* **34** (1989) 174–176.
4. Zhao, J. T.; Cenzual, K.; Parthé, E.: Monoclinic La₂AlGe₆ and isotypes, a vacancy variant of the orthorhombic SmNiGe₃ type. *Acta Crystallogr. C* **47** (1991) 1777–1781.
5. Teatum, E.; Gschneidner Jr., K. A.; Waber, J.: Rep. LA-4003. National Technical Information Service, Springfield, VA, USA 1968.
6. Sheldrick, G. M.: SHELXS-97. Program for the solution of crystal structures. University of Göttingen, Germany 1997.
7. Sheldrick, G. M.: SHELXL-97. Program for refining crystal structures. University of Göttingen, Germany 1997.
8. Gelato, L. M.; Parthé, E.: STRUCTURE TIDY - a computer program to standardize crystal structure data. *J. Appl. Crystallogr.* **20** (1987) 139–143.